Detailed Chemical Kinetics Modeling of Knock in GT-POWER

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Agenda

• Introduction
• GT-POWER v7.2 Knock Model
• Chemical Kinetic Mechanism Selection
• Parametric Studies
  – Octane Rating, EGR, Intake Temperature and Ethanol Ratio
• Comparison with Engine Knock Data
• GT-POWER v7.3 Knock Model Results
• Conclusions
Introduction

Autoignition theory is the most common explanation for the origin of knock

- Spontaneous combustion occurs in the end-gas region when fuel-air mixture is compressed to sufficiently high pressures and temperatures
- Chemistry of fuel-air oxidation plays a vital role in describing pre-flame reactions and rapid energy release at the time of autoignition

Fig 9-63 (Heywood, 1988)
Current Models for Borderline Knock

1. Peak Unburned Gas Temperature

2. Single-Reaction Induction Time Models

3. Multi-Step Chemistry
Objectives

• To develop a chemistry based spark knock model that simulates end-gas autoignition by solving multi-step chemistry of gasoline oxidation within GT-POWER

• Goal is better prediction of spark knock within the limitations of a 1-D engine model
GT-POWER 7.2 Knock Model Schematic
Knock Chamber Pressure & Temperature Matching

Cylinder Pressure (0% EGR, No ignition)

- Main Cylinder
- Knock Chamber

Knock Chamber
Main Cylinder

Unburned Zone Temperature (no EGR, No Ignition)

- Main Cylinder
- Knock Chamber
Chemical Kinetic Mechanism

• MC9 mechanism developed by Ra & Reitz at ERC, University of Wisconsin
  – Developed specifically for PRF & Ethanol oxidation
    • 46 species and 142 reactions
  – Extracted from MultiChem mechanism for multicomponent fuels described in *Combustion and Flame* 158 (2011) 69–90
  – Validated with ignition delay measurements in shock tubes and engines at T < 1600 K and P < 55 bar
  – Comparison with three other kinetic mechanisms performed at Ford showed MC9 to be the best in predicting ignition delay under knock like conditions
Parametric Studies
1000 rpm, $P_{in} = 1$ bar

- Fuel Octane Rating
  - 80 RON, 90 RON, 100 RON

- EGR
  - 0%, 30%, 45%

- Intake Temperature
  - 300 K, 330 K

- Ethanol Blend
  - E0, E20, E50, E100
Effect of Octane Rating
at 1000 rpm, 0 EGR, CA50 = 10 ATDC
Effect of Octane Rating
at 1000 rpm, 0 EGR, CA50 = 20 ATDC
Effect of Octane Rating
at 1000 rpm, 0 EGR, CA50 = 30 ATDC
Effect of EGR and Intake Temperature on Knock

• Swept CA50 (surrogate for spark timing) for 90 RON fuel at 1000 rpm to determine the impact of EGR ratio and intake temperature on autoignition
• Conducted DOE at 0%, 30%, 45% EGR and 300 K, 330 K Tin
• Defined “Knock Limited CA50” as the latest CA50 at which autoignition occurs
  – no autoignition at KLCA50 + 1° CA
Main Effects Plot

Main Effects Plot (data means) for CA50

<table>
<thead>
<tr>
<th>EGR</th>
<th>Intake Temp</th>
</tr>
</thead>
<tbody>
<tr>
<td>~4° CA50 advance / 10% EGR</td>
<td>~1° CA50 retard / 15°C increase in $T_{in}$</td>
</tr>
</tbody>
</table>

Mean of CA50 vs. EGR and Intake Temp
Effect of Ethanol Blend in Fuel

2000 RPM, 13 bar BMEP
E0 = 80 RON
CA50 = 17° ATDC
Comparison with High BMEP SCE Knock Data

2000 RPM, 18 bar NMEP EGR Sweep 0 - 25%

Data provided by Brad VanDerWege, Ford Motor Company
Knock Assessment

• Cycles evaluated
  – **Mean**
    • Burn rate specified by average CA50 and B1090 of 300 engine cycles
  – **5th percentile of fastest cycles**
    • \( CA50 = CA50_{avg} - 1.64\sigma_{CA50} \)
    • \( B1090 = B1090_{avg} - 1.64\sigma_{B1090} \)
  – **2nd percentile of fastest cycles**
    • \( CA50 = CA50_{avg} - 2\sigma_{CA50} \)
    • \( B1090 = B1090_{avg} - 2\sigma_{B1090} \)
Modeling Assumptions

• Temperature and concentration of the end gas assumed to be uniform
  – Autoignition chemistry solved at bulk unburned zone temperature
  – Model predicted knock onset will be later than reality
Modeling Procedure

1. Model Calibration (no EGR) - matched in-cylinder pressure and air flow rate by performing a DOE of intake and exhaust runner lengths at
   - measured MAP, N, Tin, CA50 (mean), B10-90 (mean), cylinder geometry, valve lift profiles/phasing, RON, cylinder head temperatures
   - used default values of wall & piston temperatures and heat transfer coefficients

2. Knock Chamber - Matched pressure, temperature and mass in the knock chamber with the unburned zone

3. Simulated Mean, 5th and 2nd percentile cycles with kinetics
   • Criteria for autoignition – alignment between autoignition time in the knock chamber and cylinder mass burn profile
Comparison to Measurements
Pressure Matching – No EGR

Intake runner = 900 mm
Exhaust runner = 950 mm
TWALL = 400 K

<table>
<thead>
<tr>
<th></th>
<th>MAP (bar)</th>
<th>Air Flow (kg/hr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Measured</td>
<td>1.59</td>
<td>50.45</td>
</tr>
<tr>
<td>Simulated</td>
<td>1.59</td>
<td>50.16</td>
</tr>
<tr>
<td>% Diff</td>
<td>0</td>
<td>-0.58</td>
</tr>
</tbody>
</table>

InCylinder Pressure at 2000 RPM, 18 bar NMEP, 0 EGR
EngCylinder part Cylinder-01

Advanced Engineering
Simulations – No EGR, Mean Cycle

CA50 = 22.1° ATDC

B1090 = 24.7°

Autoignition at 61° ATDC
Simulations – No EGR, Mean Cycle

Autoignition at 61° ATDC
Simulations – No EGR, Mean Cycle

Mean cycle will not knock

Unburned zone mass already consumed
Simulations – No EGR, 5th Percentile Cycle

CA50 = 19.4° ATDC (-2.7° from mean)
B10-90 = 21.6° (-3.1° from mean)

Autoignition at 45° ATDC
(-16° from mean)

\[ CA50 = CA50 - 1.64\sigma_{CA50} \]
\[ B10-90 = B10-90 - 1.64\sigma_{B1090} \]
Simulations – No EGR, 5th Percentile Cycle
Simulations – No EGR, 2\textsuperscript{nd} Percentile Cycle

CA50 = 18.8° ATDC (-0.6° from 5\textsuperscript{th} percentile )

B1090 = 20.9° (-0.7° from 5\textsuperscript{th} percentile)

Autoignition at 41° ATDC
(-4° from 5\textsuperscript{th} percentile)

\[
\text{CA50} = \text{CA50} - 2\sigma_{\text{CA50}}
\]

\[
\text{B10-90} = \text{B10-90} - 2\sigma_{\text{B1090}}
\]
Simulations – No EGR, 2\textsuperscript{nd} Percentile Cycle
Summary of No EGR Case

• Autoignition occurs in the mean cycle much after the unburned zone mass has been completely consumed
  – Mean cycle is not likely to knock
• For the 2\textsuperscript{nd} and 5\textsuperscript{th} percentile cycles, autoignition occurs close to the end of combustion in the main chamber
  – These cycles will likely knock in a real engine
• Occurrence of autoignition in the knock chamber close to the end of combustion will be used as the criteria to indicate knock at other operating conditions
Comparison with Measurements

EGR: 5% – 25%

• Kept all geometric and thermal variables the same
  – Intake and exhaust runner lengths
  – Wall temperature
  – Heat transfer coefficient

• CA50 and B1090 specified from measurements

• Intake temperature varied with EGR
  – 35.7°C (no EGR) to 42°C (25% EGR)

• Varied MAP to match air flow rate within 2.5% of measurements
Calibration of MAP and Air Flow for the Different EGR Cases

<table>
<thead>
<tr>
<th></th>
<th>5% EGR</th>
<th>10% EGR</th>
<th>15% EGR</th>
<th>20% EGR</th>
<th>25% EGR</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>MAP (bar)</td>
<td>Air Flow (kg/hr)</td>
<td>MAP (bar)</td>
<td>Air Flow (kg/hr)</td>
<td>MAP (bar)</td>
</tr>
<tr>
<td>Measured</td>
<td>1.65</td>
<td>49.77</td>
<td>1.72</td>
<td>49.55</td>
<td>1.76</td>
</tr>
<tr>
<td>Simulated</td>
<td>1.62</td>
<td>48.82</td>
<td>1.69</td>
<td>48.45</td>
<td>1.73</td>
</tr>
<tr>
<td>% Diff</td>
<td>-1.8</td>
<td>-1.91</td>
<td>-1.94</td>
<td>-2.22</td>
<td>-1.7</td>
</tr>
</tbody>
</table>
Comparison to Measurements
Pressure Matching – 5% EGR
Simulations – 5% EGR, Mean Cycle

Cylinder Pressure (5% EGR, Mean Cycle)

- Main Cylinder
- Knock Chamber

No Auto Ignition
Simulations – 5\% EGR, 5\textsuperscript{th} Percentile Cycle

Autoignition at 49° ATDC

CA50 = CA50 – 1.64 \sigma

B10-90 = B10-90 – 1.64\sigma
Simulations – 5\% EGR, 5\textsuperscript{th} Percentile Cycle
Simulations – 5% EGR, 2nd Percentile Cycle

Results for 10 – 25% EGR are similar
Detailed Kinetics in Unburned Zone (V7.3)

• User defined kinetics mechanism for predicting autoignition
• Kinetics reactions are active in the unburned zone during the combustion period
• Can be used with all SI combustion models (SIWiebe, SITurb, profile combustion, etc.)
• Autoignition is detected based on rate of pressure rise in the unburned zone
• Additional criterion can be used to simulate the onset of detectable knock, e.g. unburned mass fraction, knock index, etc.
KLSA & CA 50 advance vs. EGR

Model: SI Turb, Speed: 1000 rpm, BMEP 15, EGR 0-25%, Intake temperature: 300K
Maintained constant BMEP with EGR using pressure boost.
Unburned Mass Fraction at Knock Onset vs. Spark Timing

Unburned mass fraction at knock onset, 0% EGR

Spark Advance

Spark

1000 rpm, 15 bar BMEP
KLSA vs. EGR
Comparison with Experimental Data from Literature

Conclusions

• The detailed chemical kinetic mechanism used in this study was able to describe the effect of fuel chemistry and EGR ratio well on autoignition
  – Validation with single cylinder engine dyno data shows autoignition occurring towards the end of combustion with combustion phased 3 to 5° crank angle advanced of the mean cycle over the range of loads and EGR investigated
  – Mean cycle did not autoignite in any case when there was unburned mass left in the main chamber

• The chemical kinetic model provides a good trade-off between computational speed and model fidelity

• GT-POWER v7.3 incorporates knock kinetics in the main chamber, thereby eliminating the approximations made in the indirect approach used in this study
Unburned Mass Fraction at Knock Onset vs. Spark Timing

KLSA vs. Intake Temperature

Speed: 1000 rpm
BMEP: 15 bar
Pressure Traces (v 7.3)